

CO ₂	C X,1,1. O,1,r1,2,90. O,1,r1,2,90.,3,180.,0 R1= 1.16699443 ANGSTROM
CO ₂ :CO	C X,1,1. O,1,r1,2,a1 O,1,r1,2,a1,3,180.,0 C,1,r2,3,a1,2,0.,0 O,1,r3,3,a1,2,0.,0 R1= 1.16689562 ANGSTROM A1= 90.26092656 DEGREE R2= 3.18895171 ANGSTROM R3= 4.32419001 ANGSTROM
CO ₂ :HCCH	C X,1,1. O,1,r1,2,a1 O,1,r1,2,a1,3,180.,0 X,1,r2,3,a1,2,0.,0 C,5,r3,2,90.,3,0.,0 C,5,r3,2,90.,4,0.,0 H,5,r4,2,a4,3,0.,0 H,5,r4,2,a4,4,0.,0 R1= 1.16695767 ANGSTROM A1= 90.39127333 DEGREE R2= 3.20093589 ANGSTROM R3= 0.60538158 ANGSTROM R4= 1.66986445 ANGSTROM A4= 89.81599345 DEGREE
CO ₂ :NCH(T- shaped)	C X,1,1. O,1,r1,2,a1 O,1,r1,2,a1,3,180.,0 N,1,r2,3,a1,2,0.,0 C,1,r3,3,a1,2,0.,0 H,1,r4,3,a1,2,0.,0 R1= 1.16688463 ANGSTROM A1= 90.76445447 DEGREE R2= 2.96202581 ANGSTROM R3= 4.12143255 ANGSTROM R4= 5.18937839 ANGSTROM

CO ₂ -HCN (linear, H-bonded)	C X,1,1. O,1,R1,2,90. O,1,R2,2,90.,3,180.,0 H,1,R3,2,90.,3,180.,0 X,5,1.,1,90.,2,0.,0 C,5,R4,6,90.,1,180.,0 N,5,R5,6,90.,1,180.,0 R1= 1.16368133 ANGSTROM R2= 1.16904557 ANGSTROM R3= 3.39974308 ANGSTROM R4= 1.06848510 ANGSTROM R5= 2.22872961 ANGSTROM CCSD(T)/CBS energy= -281.741349260795 Hartree (1.3 kJ/mol less stable than the T shaped structure)
CO ₂ :NH ₃	C X,1,1. O,1,r1,2,90. O,1,r2,2,a1,3,180.,0 N,1,r3,3,a3,2,0.,0 H,5,r4,1,a4,3,180.,0 H,5,r5,1,a5,3,d5,0 H,5,r5,1,a5,3,-d5,0 R1= 1.16703785 ANGSTROM R2= 1.16719581 ANGSTROM A1= 92.59741743 DEGREE R3= 2.92218508 ANGSTROM A3= 91.62419041 DEGREE R4= 1.01517012 ANGSTROM A4= 110.97260314 DEGREE R5= 1.01524170 ANGSTROM A5= 113.09898728 DEGREE D5= 60.39689047 DEGREE
CO ₂ :OH ₂	C X,1,1. O,1,r1,2,a1 O,1,r1,2,a1,3,180.,0 O,1,r2,3,a1,2,0.,0 H,5,r3,1,a3,3,0.,0

	H,5,r3,1,a3,4,0.,0 R1= 1.16688256 ANGSTROM A1= 90.94990727 DEGREE R2= 2.75775306 ANGSTROM R3= 0.96167110 ANGSTROM A3= 127.62334371 DEGREE
CO ₂ :PH ₃	C X,1,1. O,1,r1,2,90. O,1,r2,2,a1,3,180.,0 P,1,r3,2,a3,3,0.,0 H,5,r4,1,a4,3,180.,0 H,5,r5,1,a5,3,d5,0 H,5,r5,1,a5,3,-d5,0 R1= 1.16744332 ANGSTROM R2= 1.16664608 ANGSTROM A1= 90.78332173 DEGREE R3= 3.52758267 ANGSTROM A3= 4.49836564 DEGREE R4= 1.41846385 ANGSTROM A4= 136.64671037 DEGREE R5= 1.41870649 ANGSTROM A5= 114.69537750 DEGREE D5= 53.45250399 DEGREE
CO ₂ :SH ₂	C X,1,1. O,1,r1,2,a1 O,1,r1,2,a1,3,180.,0 S,1,r2,3,a1,2,0.,0 H,5,r3,1,a3,3,d3,0 H,5,r3,1,a3,4,-d3,0 R1= 1.16703609 ANGSTROM A1= 90.47410791 DEGREE R2= 3.42489299 ANGSTROM R3= 1.34213053 ANGSTROM A3= 96.11653785 DEGREE D3= 43.40684932 DEGREE

N ₂ O	N X 1 1. N 1 r1 2 90. O 1 r2 2 90. 3 180. R1= 1.13266309 ANGSTROM R2= 1.19119506 ANGSTROM
N ₂ O:CO	N X 1 1. N 1 r1 2 90. O 1 r2 2 a2 3 180. C 1 r3 3 a3 2 180. X 5 1. 1 90. 3 0. O 5 r4 6 a4 1 180. R1= 1.13210638 ANGSTROM R2= 1.19095036 ANGSTROM A2= 90.12864491 DEGREE R3= 3.17630540 ANGSTROM A3= 94.90525654 DEGREE R4= 1.13540183 ANGSTROM A4= 99.78237333 DEGREE
N ₂ O:HCCH	N X 1 1. N 1 B2 2 90. O 1 B3 2 A2 3 180. X 1 B4 3 A3 2 0. C 5 B5 1 A4 3 0. C 5 B5 1 A5 4 0. H 5 B7 1 A6 3 0. H 5 B8 1 A7 4 0. B2= 1.13191032 ANGSTROM B3= 1.19074773 ANGSTROM A2= 89.80799318 DEGREE B4= 3.22197129 ANGSTROM A3= 92.38294855 DEGREE B5= 0.60539272 ANGSTROM A4= 93.04456666 DEGREE A5= 86.24445372 DEGREE B7= 1.66979961 ANGSTROM A6= 93.34146896 DEGREE B8= 1.66974609 ANGSTROM A7= 86.18314121 DEGREE
N ₂ O:NCH	N X 1 1. N 1 r1 2 90. O 1 r2 2 a2 3 180. N 1 r3 3 a3 2 180.

	X 5 1. 1 90. 3 0. C 5 r4 6 a4 1 180. H 5 r5 6 a5 1 180. R1= 1.13178957 ANGSTROM R2= 1.19055736 ANGSTROM A2= 89.70319317 DEGREE R3= 3.00237128 ANGSTROM A3= 92.51860891 DEGREE R4= 1.15957570 ANGSTROM A4= 97.69934838 DEGREE R5= 2.22743057 ANGSTROM A5= 97.72652993 DEGREE
N ₂ O:OH ₂	N X 1 1. N 1 r1 2 90. O 1 r2 2 a2 3 180. O 1 r3 3 a3 2 180. H 5 r4 1 a4 3 0. H 5 r5 1 a5 4 0. R1= 1.13038009 ANGSTROM R2= 1.19356294 ANGSTROM A2= 89.58216709 DEGREE R3= 2.85478673 ANGSTROM A3= 100.63604826 DEGREE R4= 0.96132692 ANGSTROM A4= 171.06312463 DEGREE R5= 0.96229856 ANGSTROM A5= 84.16208585 DEGREE
N ₂ O:SH ₂	N X 1 1. N 1 r1 2 90. O 1 r2 2 a2 3 180. S 1 r3 3 a3 2 180. H 5 r4 1 a4 3 d4 H 5 r5 1 a5 4 d5 R1= 1.13165091 ANGSTROM R2= 1.19211561 ANGSTROM A2= 90.03095303 DEGREE R3= 3.44374168 ANGSTROM A3= 100.17649793 DEGREE R4= 1.34202505 ANGSTROM A4= 116.84829282 DEGREE D4= 54.89834523 DEGREE R5= 1.34199764 ANGSTROM A5= 79.01178960 DEGREE D5= -37.76856958 DEGREE
N ₂ O:NH ₃	N

	<p>X 1 1. N 1 r1 2 90. O 1 r2 2 a2 3 180. N 1 r3 3 a3 2 180. H 5 r4 1 a4 3 0. H 5 r5 1 a5 4 d5 H 5 r5 1 a5 4 -d5</p> <p>R1= 1.13098877 ANGSTROM R2= 1.19179889 ANGSTROM A2= 89.55023730 DEGREE R3= 3.02111852 ANGSTROM A3= 97.84862436 DEGREE R4= 1.01499854 ANGSTROM A4= 137.70190324 DEGREE R5= 1.01534736 ANGSTROM A5= 98.49788997 DEGREE D5= 53.86846339 DEGREE</p>
N ₂ O:PH ₃	<p>N X 1 1. N 1 r1 2 90. O 1 r2 2 a2 3 180. P 1 r3 3 a3 2 180. H 5 r4 1 a4 3 180. H 5 r5 1 a5 4 d5 H 5 r5 1 a5 4 -d5</p> <p>R1= 1.13171135 ANGSTROM R2= 1.19246557 ANGSTROM A2= 90.14148022 DEGREE R3= 3.47922869 ANGSTROM A3= 106.98783124 DEGREE R4= 1.41889443 ANGSTROM A4= 194.97926109 DEGREE R5= 1.41867129 ANGSTROM A5= 96.33357103 DEGREE D5= 47.21461949 DEGREE</p>

CS ₂	C X,1,1. S,1,r1,2,90. S,1,r1,2,90.,3,180.,0 } R1= 1.56547025 ANGSTROM
CS ₂ :CO	C X,1,1. S,1,r1,2,90. S,1,r2,2,90.,3,180.,0 C,1,r3,2,90.,4,0.,0 O,1,r4,2,90.,4,0.,0 R1= 1.56626815 ANGSTROM R2= 1.56588685 ANGSTROM R3= 5.08860843 ANGSTROM R4= 6.22423311 ANGSTROM
CS ₂ :HCCH	C X,1,1. S,1,r1,2,90. S,1,r2,2,90.,3,180.,0 X,1,r3,2,90.,4,0.,0 C,5,r4,1,90.,2,0.,0 C,5,r4,1,90.,2,180.,0 H,5,r5,1,a5,2,0.,0 H,5,r5,1,a5,2,180.,0 R1= 1.56672045 ANGSTROM R2= 1.56590668 ANGSTROM R3= 5.13418872 ANGSTROM R4= 0.60526361 ANGSTROM R5= 1.66965346 ANGSTROM A5= 90.01235305 DEGREE
CS ₂ :NCH	C X,1,1. S,1,r1,2,90. S,1,r2,2,90.,3,180.,0 N,1,r3,2,90.,4,0.,0 C,1,r4,2,90.,4,0.,0 H,1,r5,2,90.,4,0.,0 R1= 1.56903001 ANGSTROM R2= 1.56449571 ANGSTROM R3= 4.84933103 ANGSTROM R4= 6.00908780 ANGSTROM R5= 7.07712244 ANGSTROM
CS ₂ :NH ₃	C X,1,1. S,1,r1,2,90.

	S,1,r2,2,90.,3,180.,0 N,1,r3,2,90.,4,0.,0 H,5,r4,1,a4,2,0.,0 H,5,r4,1,a4,2,120.,0 H,5,r4,1,a4,2,-120.,0 R1= 1.56927998 ANGSTROM R2= 1.56557077 ANGSTROM R3= 4.86960043 ANGSTROM R4= 1.01526978 ANGSTROM A4= 112.46411542 DEGREE
CS ₂ :OH ₂	C X,1,1. S,1,r1,2,90. S,1,r2,2,90.,3,180. O,1,r3,2,90.,4,0. H,5,r4,1,a4,2,0. H,5,r4,1,a4,2,180. R1= 1.56908753 ANGSTROM R2= 1.56474300 ANGSTROM R3= 4.69698267 ANGSTROM R4= 0.96186448 ANGSTROM A4= 127.83925153 DEGREE
CS ₂ :PH ₃	C X,1,1. S,1,r1,2,90. S,1,r2,2,a1,3,180.,0 P,1,r3,2,a3,3,0.,0 H,5,r4,1,a4,3,180.,0 H,5,r5,1,a5,3,d5,0 H,5,r5,1,a5,3,-d5,0 R1= 1.56556725 ANGSTROM R2= 1.56539052 ANGSTROM A1= 89.42702346 DEGREE R3= 3.79373352 ANGSTROM A3= 11.75237846 DEGREE R4= 1.42033793 ANGSTROM A4= 128.90473280 DEGREE R5= 1.41988053 ANGSTROM A5= 55.17376969 DEGREE D5= 117.62108257 DEGREE
CS ₂ :SH ₂	C X,1,1. S,1,r1,2,90. S,1,r2,2,90.,3,180.,0 S,1,r3,2,a3,4,0.,0 H,5,r4,1,a4,2,d4,0 H,5,r4,1,a4,2,-d4,0

	R1=	1.56670591 ANGSTROM
	R2=	1.56608708 ANGSTROM
	R3=	5.32695751 ANGSTROM
	A3=	95.98545593 DEGREE
	R4=	1.34227372 ANGSTROM
	A4=	83.64947707 DEGREE
	D4=	133.48813863 DEGREE